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Recent Developments in Toxico-Cheminformatics and Progress Towards a New Paradigm for Predictive Toxicology

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EPA's National Center for Computational Toxicology is building capabilities to support a new paradigm for toxicity screening and prediction through harnessing of legacy toxicity data, creation of data linkages, and generation of new in vitro screening data. In association with EPA's ToxCast™, ToxRef DB, and ACToR projects, the DSSTox project provides cheminformatics support and is improving public access to structure-annotated chemical toxicity information to facilitate modeling, data-mining and read-across approaches. DSSTox enables linkages between previously isolated toxicity data resources associated with environmental and industrial chemicals, such as microarray databases, and all DSSTox content has been integrated into PubChem. Phase I of the ToxCast™ project has generated high-throughput screening (HTS) data for a set of 320 chemicals, mostly pesticide actives with rich toxicology profiles. Presenters at the first ToxCast Data Analysis Summit were provided early access to these data and reported on the challenges posed by the data, as well as promising avenues for investigation. Incorporating traditional SAR concepts into this new HTS data-rich world poses conceptual and practical challenges, but also holds great promise for improving predictive capabilities. *This work was reviewed by EPA and approved for publication, but does not necessarily reflect EPA policy.*